

Molecular Dipole Moments and Lattice Energies from Accurate X-ray Data

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Beamline(s): X3A1

Dipole Moments: Highly accurate X-ray data can be used to evaluate molecular dipole moments in the solid state. Some results, based on data collected at X3A1 and summarized in **Table 1**, show a systematic increase compared with isolated molecule values, and thus give evidence for the effect of induced polarization of the molecules due to the crystalline environment. Parallel theoretical calculations on periodic crystals (not reported here) provide supporting evidence. The polarization must be taken into account in force fields used for calculation of molecular polarization and crystal lattice energies.

Table 1. Solid state molecular dipole moments from 20K Synchrotron Diffraction and theoretical isolated-molecule values (from large basis-set DFT calculations)

Molecule	<i>isolated molecule</i> (Debye)	<i>molecule in crystal</i> (Debye)
<i>p</i> -nitroaniline	8.0	12.3(10)
<i>p</i> -amino <i>p</i> '-nitrobiphenyl	9.2	23.8(42)
glycylglycine	23.2	27.8(17)
Boc-Gln-D-Iva-Hyp-Ala-Phol	13.4	29.5

Lattice Energies: Electrostatic contribution to molecular interactions and lattice energies has been derived from the experimental densities. Results are quite encouraging and in good agreement with calorimetric lattice energies, where available, and, to the extent possible, with calculations on molecular dimers, which neglect many body interactions in the crystals (Abramov *et al.* 2000).

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References: Y.A. Abramov, A. Volkov, G. Wu, P. Coppens, *J. Phys. Chem. B*, **104**, 2183, 2000.